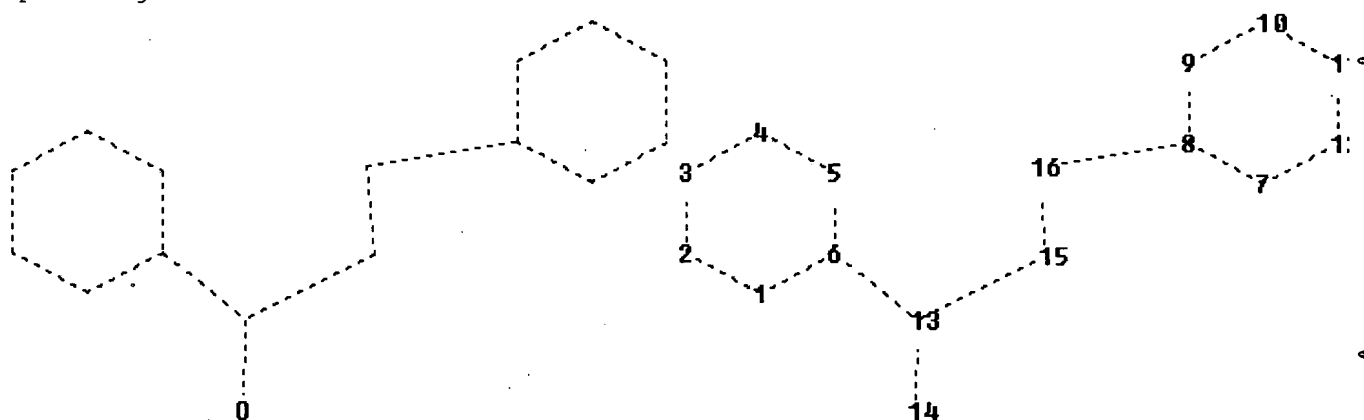Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str

chain nodes :
13   14   15   16
ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12
chain bonds :
6-13   8-16   13-14   13-15   15-16
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12
exact/norm bonds :
1-2   1-6   2-3   3-4   4-5   5-6   6-13   7-8   7-12   8-9   8-16   9-10   10-11   11-12   13-14
13-15   15-16

Connectivity :
1:3 X maximum RC ring/chain   2:3 X maximum RC ring/chain   3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain   5:3 X maximum RC ring/chain   6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain   8:3 E exact RC ring/chain   9:3 X maximum RC ring/chain   10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain   12:3 X maximum RC ring/chain   13:3 E exact RC
ring/chain   14:1
E exact RC ring/chain   15:3 X maximum RC ring/chain   16:3 X maximum RC ring/chain
Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
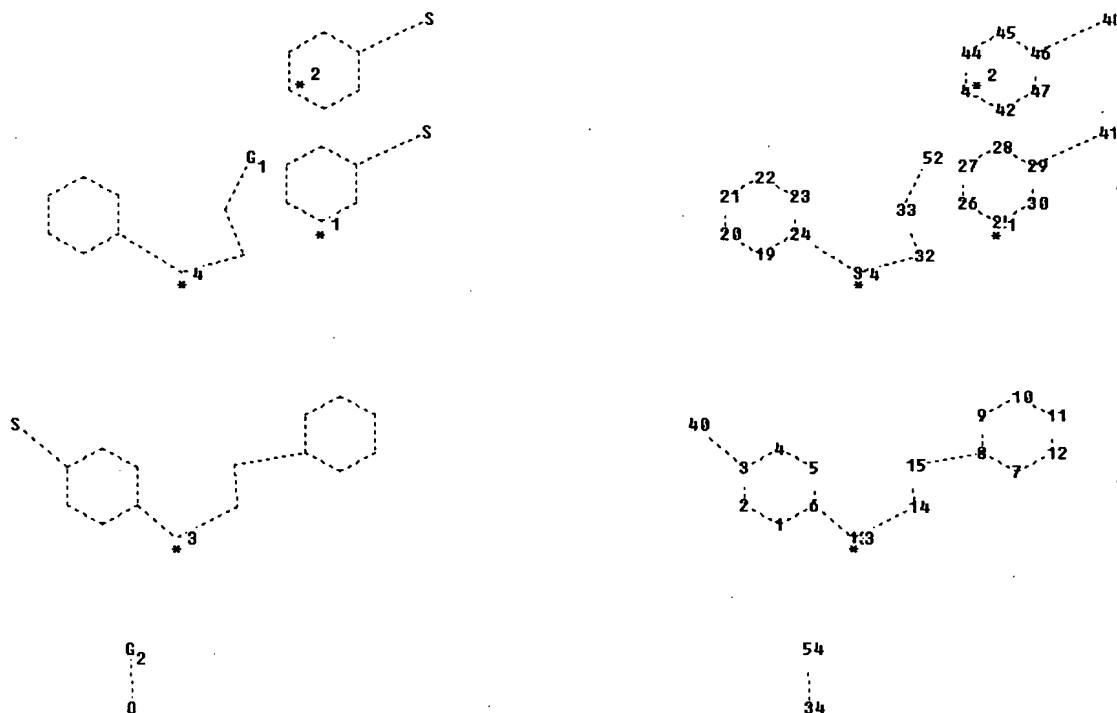11:Atom   12:Atom   13:CLASS   14:CLASS   15:CLASS   16:CLASS

L3   STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L3.str

chain nodes :
13 14 15 31 32 33 34 40 41 48 52 54
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47
chain bonds :
3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-
21
21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46
46-47
exact/norm bonds :
1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27
27-28 28-29

29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
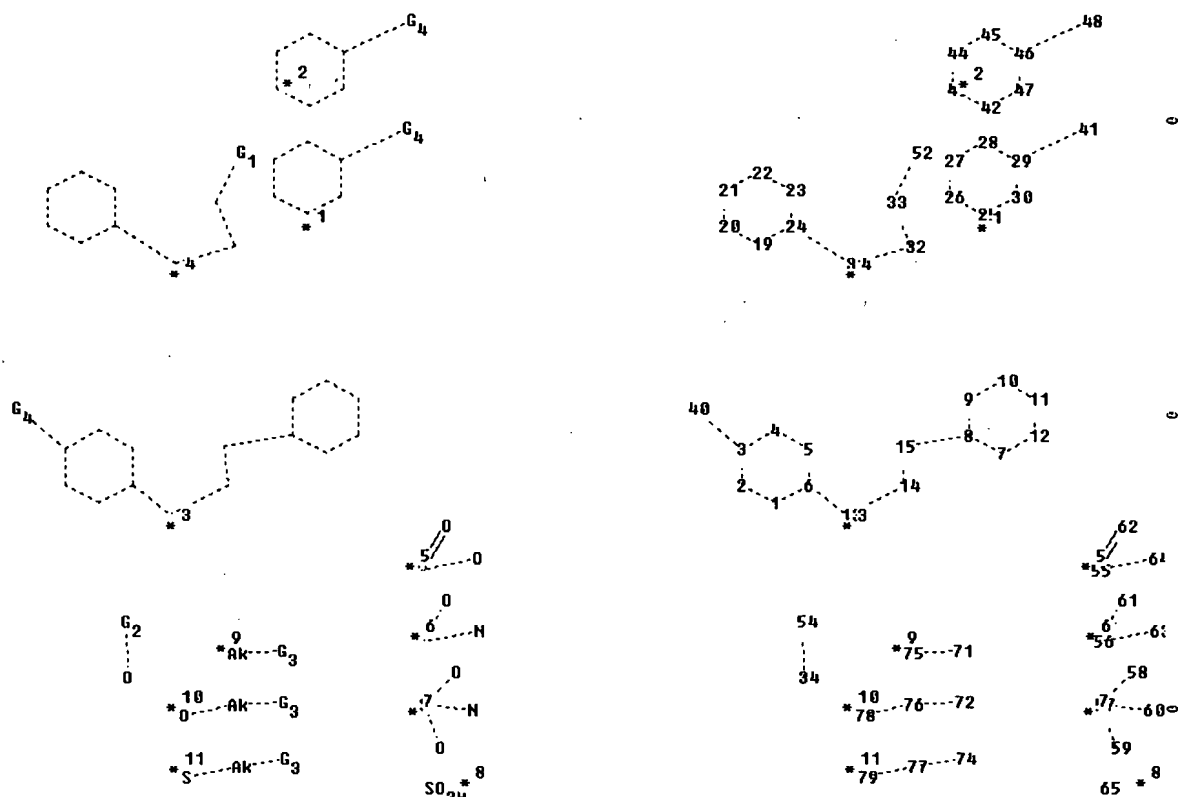46-48

G1:[*1],[*2]

G2:[*3],[*4]

Connectivity :
1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS

L5   2322 SEA FILE=REGISTRY SSS FUL L3 AND L1
L6   STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation:
Uploading L6.str

G4

*2

G1

G4

*1

*4

45 48
44 46
*2 47
42
28 41
52 27 29
21 22 23 26 30
20 24 *21
19 3 4 32
*

G4

*3

40 10
9 11
3 4 5 15 8 7 12
2 14
1 6 13
*

O
5
* O
O

G2
0

9
*Ak G3

O
6
* N

O
0
10
*O Ak G3

O
7
* N

O
11
*S Ak G3

SO3H *8

54
34

62
5
*55 61

61
6
*56 63

9
*75 71

58
10
*78 76 72

77 60
*

59
11
*79 77 74

65 *8

chain nodes :
13   14   15   31   32   33   34   40   41   48   52   54   55   56   57   58   59   61   62   64   65
71   72   74   75   76   77   78   79
ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12   19   20   21   22   23   24   25   26   27   28   29
30   42   43   44   45   46   47
ring/chain nodes :
60   63
chain bonds :
3-40   6-13   8-15   13-14   14-15   24-31   29-41   31-32   32-33   33-52   34-54   46-48
55-62   55-64   56-61   56-63   57-58   57-59   57-60   71-75   72-76   74-77   76-78   77-79
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   19-20   19-24   20-
21
21-22   22-23   23-24   25-26   25-30   26-27   27-28   28-29   29-30   42-43   42-47   43-44
44-45   45-46
46-47
exact/norm bonds :
1-2   1-6   2-3   3-4   3-40   4-5   5-6   6-13   7-8   7-12   8-9   8-15   9-10   10-11   11-12
13-14   14-15   19-20   19-24   20-21   21-22   22-23   23-24   24-31   25-26   25-30   26-27
27-28   28-29
29-30   29-41   31-32   32-33   33-52   34-54   42-43   42-47   43-44   44-45   45-46   46-47
46-48   55-62
55-64   56-61   56-63   57-58   57-59   57-60   71-75   72-76   74-77   76-78   77-79

G1:[*1],[*2]

5

G2:[*3],[*4]

G3:[*5],[*6],[*7],[*8]

G4:[*9],[*10],[*11]

Connectivity :
1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS
55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS
63:CLASS 64:CLASS
65:CLASS 71:CLASS 72:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS
79:CLASS

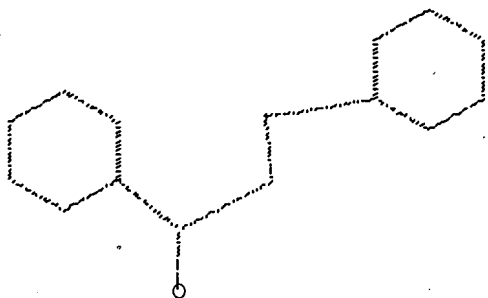
L8   68 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
L9   12 SEA FILE=ZCAPLUS ABB=ON   PLU=ON L8
L18   2 SEA FILE=ZCAPLUS ABB=ON   PLU=ON US2005-520079 /APPS
L19   2 SEA FILE=ZCAPLUS ABB=ON   PLU=ON L18 AND L9

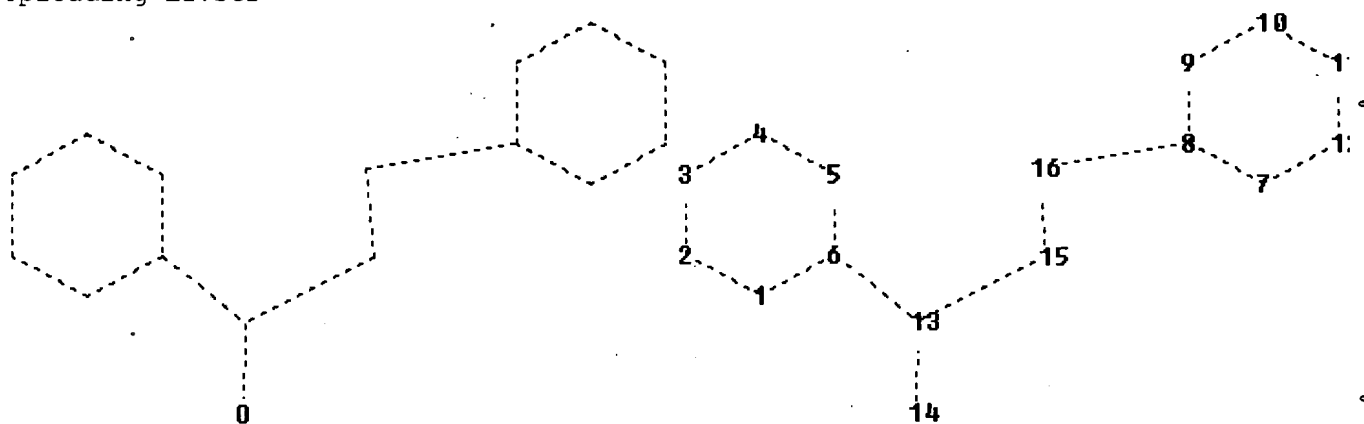=> d stat que L23
L20   38 SEA FILE=ZCAPLUS ABB=ON   PLU=ON NAJIB J?/AU
L21   70 SEA FILE=ZCAPLUS ABB=ON   PLU=ON CAUMONT K?/AU OR BERTRAND
               K?/AU
L22   11 SEA FILE=ZCAPLUS ABB=ON   PLU=ON CAUMONT B?/AU
L23   5 SEA FILE=ZCAPLUS ABB=ON   PLU=ON L20 AND (L21 OR L22)

=> d stat que L24
L1   STR

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str


```
chain nodes :
13  14  15  16
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12
chain bonds :
6-13  8-16  13-14  13-15  15-16
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  6-13  7-8  7-12  8-9  8-16  9-10  10-11  11-12  13-14
13-15  15-16
```

Connectivity :
1:3 X maximum RC ring/chain   2:3 X maximum RC ring/chain   3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain   5:3 X maximum RC ring/chain   6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain   8:3 E exact RC ring/chain   9:3 X maximum RC ring/chain   10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain   12:3 X maximum RC ring/chain   13:3 E exact RC
ring/chain   14:1
E exact RC ring/chain   15:3 X maximum RC ring/chain   16:3 X maximum RC ring/chain
Match level :
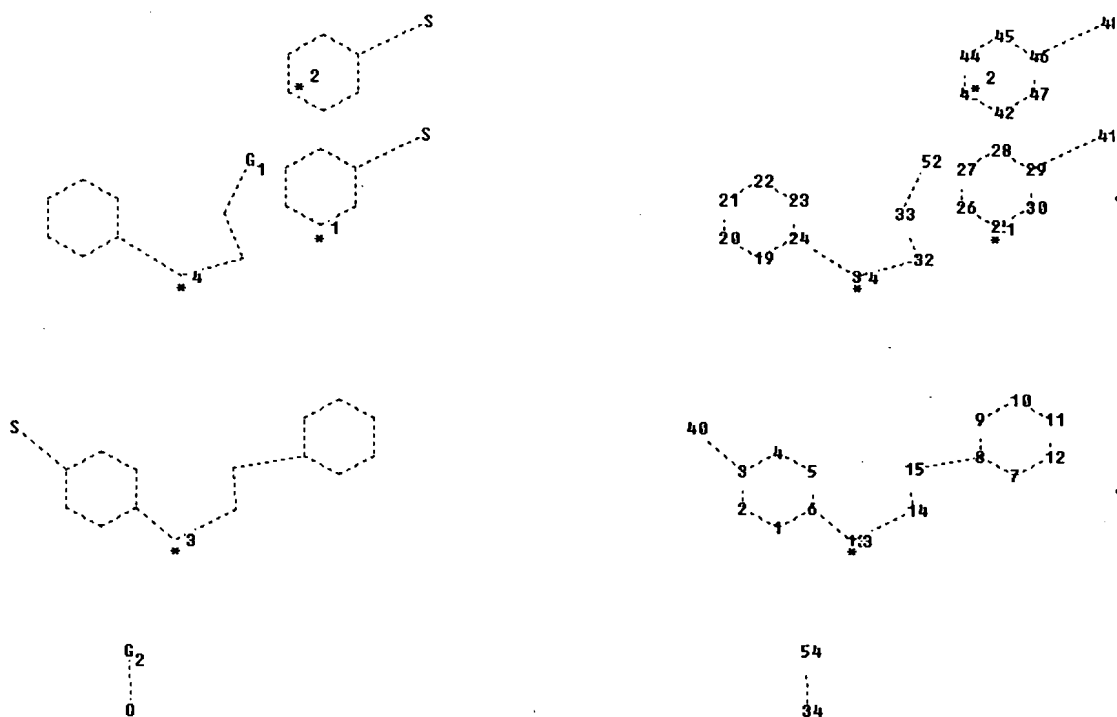1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom

11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS

L3   STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L3.str

chain nodes :
13   14   15   31   32   33   34   40   41   48   52   54
ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12   19   20   21   22   23   24   25   26   27   28   29
30   42   43   44   45   46   47
chain bonds :
3-40   6-13   8-15   13-14   14-15   24-31   29-41   31-32   32-33   33-52   34-54   46-48

ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   19-20   19-24   20-
21
21-22   22-23   23-24   25-26   25-30   26-27   27-28   28-29   29-30   42-43   42-47   43-44
44-45   45-46
46-47
exact/norm bonds :
1-2   1-6   2-3   3-4   3-40   4-5   5-6   6-13   7-8   7-12   8-9   8-15   9-10   10-11   11-12
13-14   14-15   19-20   19-24   20-21   21-22   22-23   23-24   24-31   25-26   25-30   26-27

27-28 28-29
29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
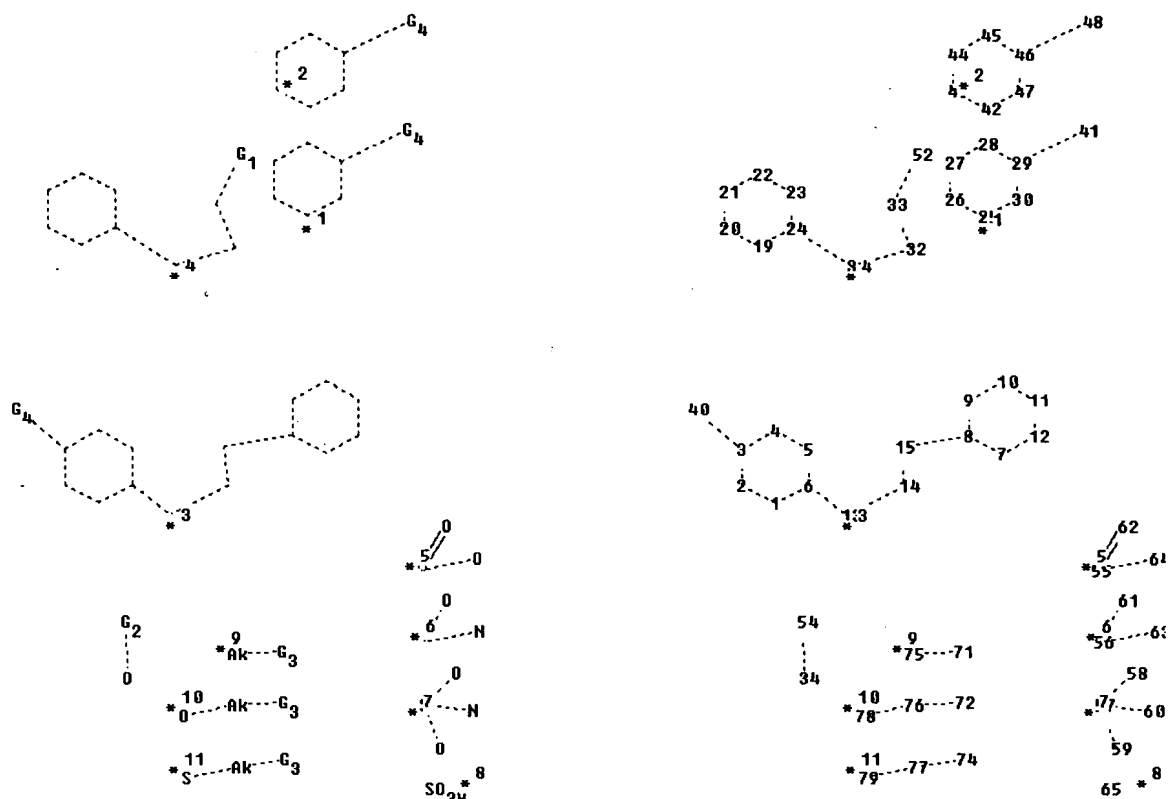46-48

G1:[*1],[*2]

G2:[*3],[*4]

Connectivity :
1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS

L5   2322 SEA FILE=REGISTRY SSS FUL L3 AND L1
L6   STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation:
Uploading L6.str

```
chain nodes :
13   14   15   31   32   33   34   40   41   48   52   54   55   56   57   58   59   61   62   64   65
71   72   74   75   76   77   78   79
ring nodes :
1    2    3    4    5    6    7    8    9    10   11   12   19   20   '21  22   23   24   25   26   27  .28  29
30   42   43   44   45   46   47
ring/chain nodes :
60   63
chain bonds :
3-40   6-13   8-15   13-14   14-15   24-31   29-41   31-32   32-33   33-52   34-54   46-48
55-62   55-64   56-61   56-63   57-58   57-59   57-60   71-75   72-76   74-77   76-78   77-79
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   19-20   19-24   20-
21
21-22   22-23   23-24   25-26   25-30   26-27   27-28   28-29   29-30   42-43   42-47   43-44
44-45   45-46
46-47
exact/norm bonds :
1-2   1-6   2-3   3-4   3-40   4-5   5-6   6-13   7-8   7-12   8-9   8-15   9-10   10-11   11-12
13-14   14-15   19-20   19-24   20-21   21-22   22-23   23-24   24-31   25-26   25-30   26-27
27-28   28-29
29-30   29-41   31-32   32-33   33-52   34-54   42-43   42-47   43-44   44-45   45-46   46-47
46-48   55-62
55-64   56-61   56-63   57-58   57-59   57-60   71-75   72-76   74-77   76-78   77-79


G1:[*1],[*2]
```

```
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FILE COVERS 1907 - 1 Oct 2007  VOL 147 ISS 15
FILE LAST UPDATED: 30 Sep 2007   (20070930/ED)

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   This file contains CAS Registry Numbers for easy and accurate
   substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L19
L1                STR
```
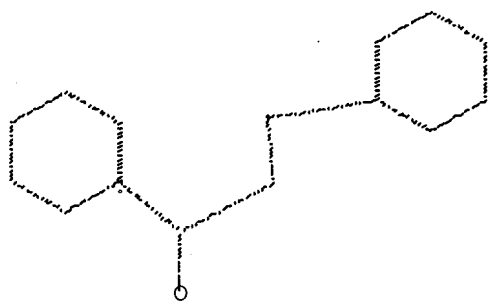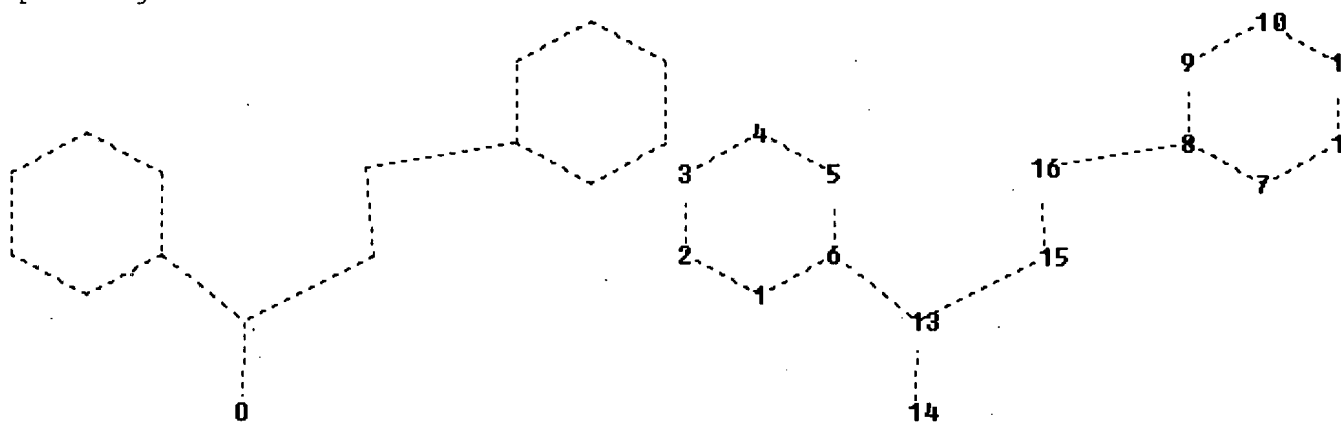
Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str

chain nodes :
13 14 15 16
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
6-13 8-16 13-14 13-15 15-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 6-13 7-8 7-12 8-9 8-16 9-10 10-11 11-12 13-14
13-15 15-16

Connectivity :
1:3 X maximum RC ring/chain   2:3 X maximum RC ring/chain   3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain   5:3 X maximum RC ring/chain   6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain   8:3 E exact RC ring/chain   9:3 X maximum RC ring/chain   10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain   12:3 X maximum RC ring/chain   13:3 E exact RC
ring/chain   14:1
E exact RC ring/chain   15:3 X maximum RC ring/chain   16:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
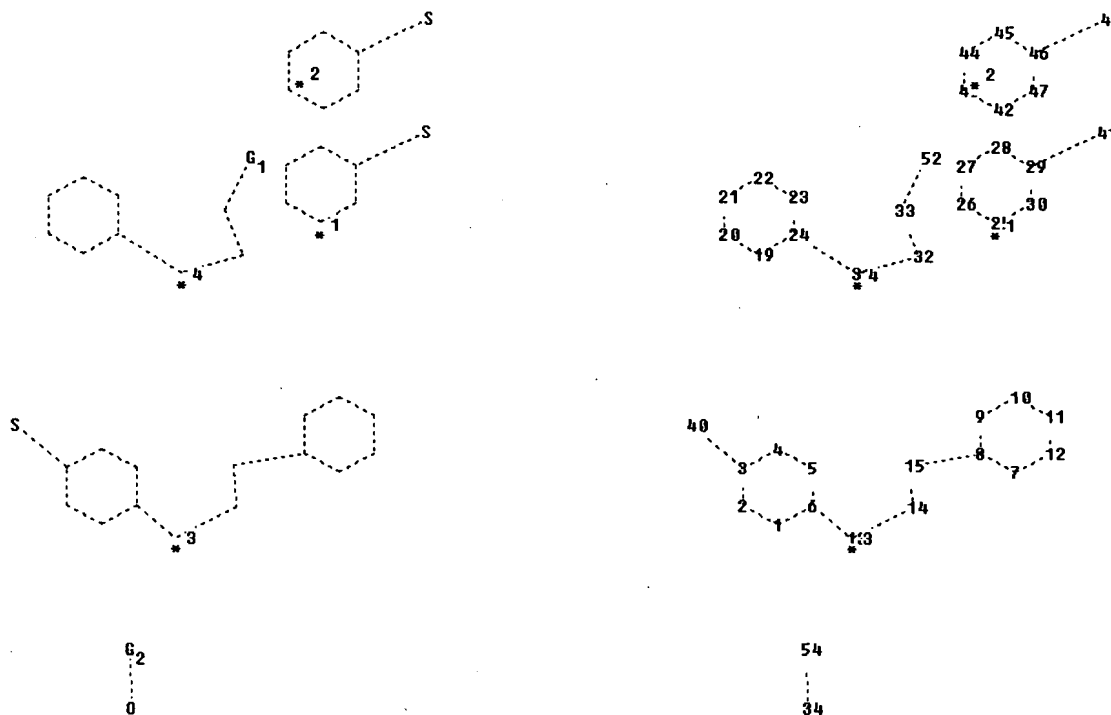11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS

L3   STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L3.str

chain nodes :
13   14   15   31   32   33   34   40   41   48   52   54
ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12   19   20   21   22   23   24   25   26   27   28   29
30   42   43   44   45   46   47
chain bonds :
3-40   6-13   8-15   13-14   14-15   24-31   29-41   31-32   32-33   33-52   34-54   46-48

ring bonds :
1-2   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   19-20   19-24   20-
21
21-22   22-23   23-24   25-26   25-30   26-27   27-28   28-29   29-30   42-43   42-47   43-44
44-45   45-46
46-47
exact/norm bonds :
1-2   1-6   2-3   3-4   3-40   4-5   5-6   6-13   7-8   7-12   8-9   8-15   9-10   10-11   11-12
13-14   14-15   19-20   19-24   20-21   21-22   22-23   23-24   24-31   25-26   25-30   26-27
27-28   28-29

30

29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
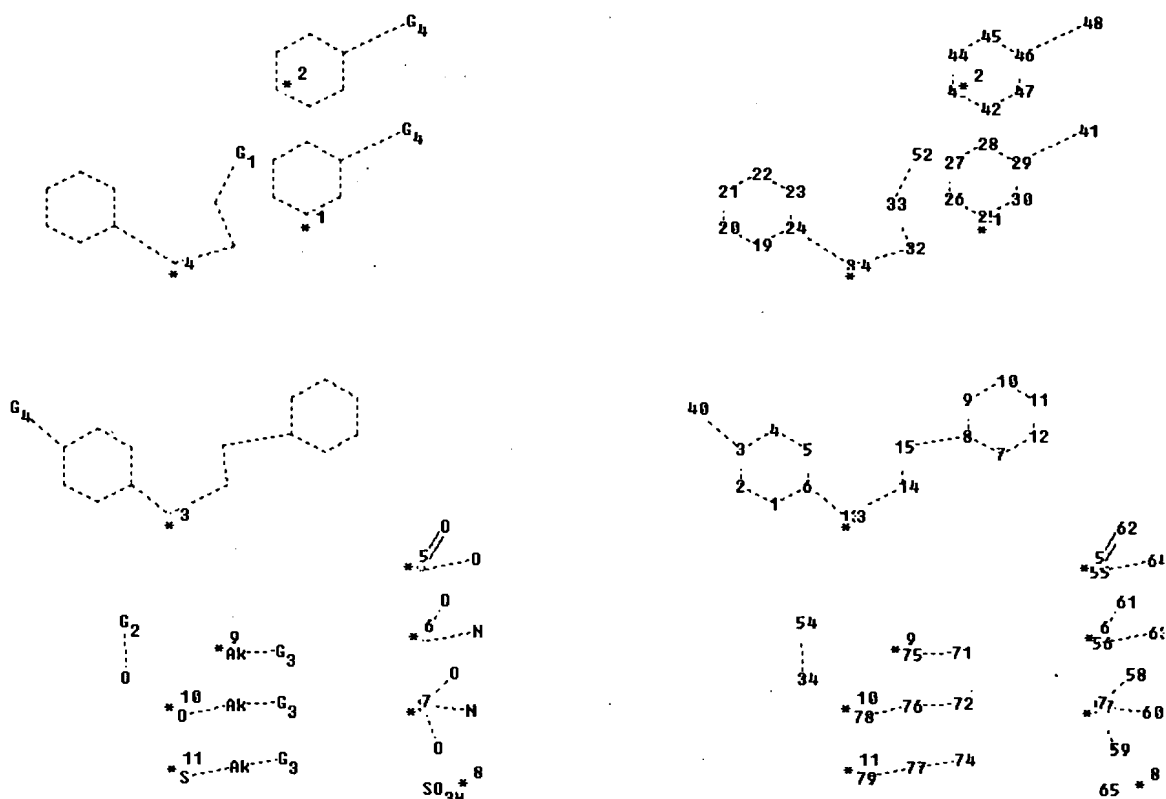46-48

G1:[*1],[*2]

G2:[*3],[*4]

Connectivity :
1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS

L5   2322 SEA FILE=REGISTRY SSS FUL L3 AND L1
L6   STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation:
Uploading L6.str

chain nodes :
13 14 15 31 32 33 34 40 41 48 52 54 55 56 57 58 59 61 62 64 65
71 72 74 75 76 77 78 79
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47
ring/chain nodes :
60 63
chain bonds :
3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48
55-62 55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21
21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46
46-47
exact/norm bonds :
1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27
27-28 28-29
29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
46-48 55-62
55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

G1:[*1],[*2]

G2:[*3],[*4]

G3:[*5],[*6],[*7],[*8]

G4:[*9],·[*10],[*11]

Connectivity :
1:3 X maximum RC ring/chain   2:3 X maximum RC ring/chain   3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain   5:3 X maximum RC ring/chain   6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain   8:3 E exact RC ring/chain   9:3 X maximum RC ring/chain   10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain   12:3 X maximum RC ring/chain   13:3 E exact RC
ring/chain   14:3
X maximum RC ring/chain   15:3 X maximum RC ring/chain   19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain   21:3 X maximum RC ring/chain   22:3 X maximum RC ring/chain   23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain   25:3 X maximum RC ring/chain   26:3 X maximum RC
ring/chain   27:3
X maximum RC ring/chain   28:3 X maximum RC ring/chain   29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain   31:3 E exact RC ring/chain   32:3 X maximum RC ring/chain   33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain   42:3 X maximum RC ring/chain   43:3 X maximum RC
ring/chain   44:3
X maximum RC ring/chain   45:3 X maximum RC ring/chain   47:3 X maximum RC ring/chain
Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:CLASS   14:CLASS   15:CLASS   19:CLASS   20:Atom   21:Atom   22:Atom
23:Atom   24:Atom
25:Atom   26:Atom   27:Atom   28:Atom   29:Atom   30:Atom   31:CLASS   32:CLASS   33:CLASS
34:CLASS   40:CLASS
41:CLASS   42:Atom   43:Atom   44:Atom   45:Atom   46:Atom   47:Atom   48:CLASS   52:CLASS
54:CLASS
55:CLASS   56:CLASS   57:CLASS   58:CLASS   59:CLASS   60:CLASS   61:CLASS   62:CLASS
63:CLASS   64:CLASS
65:CLASS   71:CLASS   72:CLASS   74:CLASS   75:CLASS   76:CLASS   77:CLASS   78:CLASS
79:CLASS

L8   68 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
L9   12 SEA FILE=ZCAPLUS ABB=ON   PLU=ON   L8

=> s L9 not L25
L26   9 L9 NOT L25

=> file beilstein
FILE 'BEILSTEIN' ENTERED AT 13:15:02 ON 01 OCT 2007
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FILE LAST UPDATED ON September 26, 2007

FILE COVERS 1771 TO 2007.
*** FILE CONTAINS 10.119,480   SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions). A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
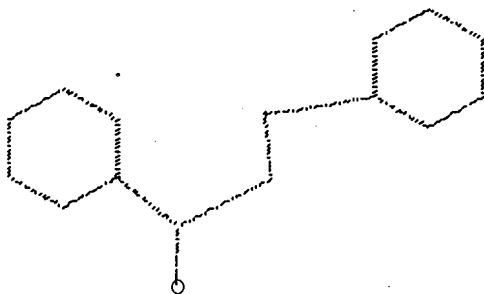   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

```
**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.               *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE  *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE         *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                       *
* FOR PRICE INFORMATION SEE HELP COST                               *
**********************************************************************
    NEW
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
  SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
  ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
  COMPOUND AT A GLANCE.
```
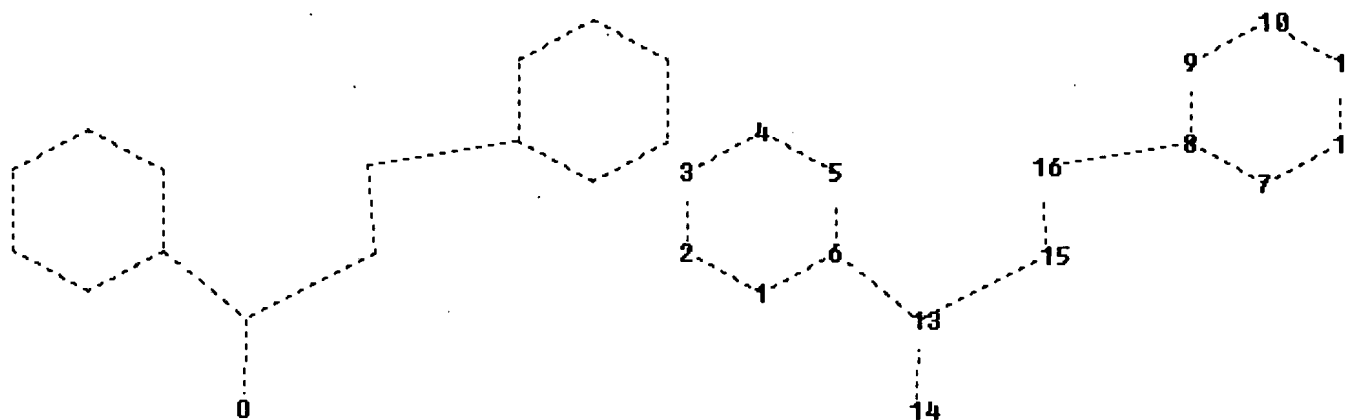
```
=> d stat que L13
L1              STR
```


Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str

```
chain nodes :
13  14  15  16
ring nodes :
1   2   3   4   5   6   7   8   9   10  11  12
chain bonds :
6-13  8-16  13-14  13-15  15-16
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  6-13  7-8  7-12  8-9  8-16  9-10  10-11  11-12  13-14
13-15  15-16
```

```
Connectivity :
1:3 X maximum RC ring/chain   2:3 X maximum RC ring/chain   3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain   5:3 X maximum RC ring/chain   6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain   8:3 E exact RC ring/chain   9:3 X maximum RC ring/chain   10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain   12:3 X maximum RC ring/chain   13:3 E exact RC
ring/chain   14:1
E exact RC ring/chain   15:3 X maximum RC ring/chain   16:3 X maximum RC ring/chain
Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:CLASS   14:CLASS   15:CLASS   16:CLASS
```
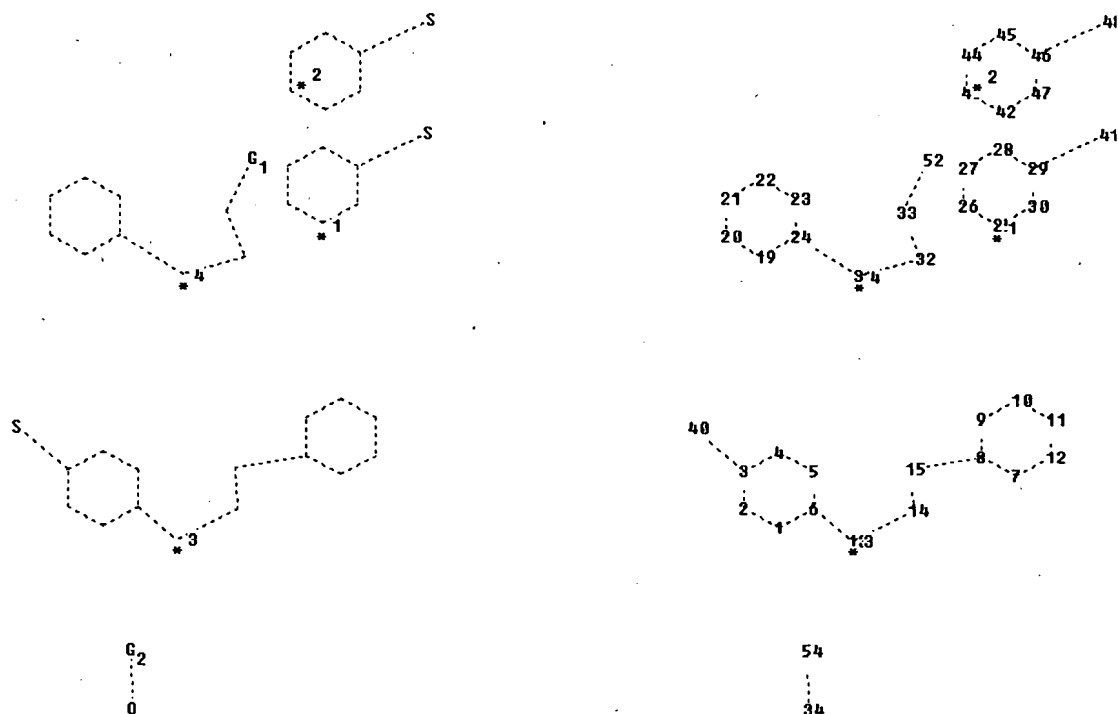
L3   STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -   AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L3.str

chain nodes :
13 14 15 31 32 33 34 40 41 48 52 54
ring nodes :
1   2   3   4   5   6   7   8   9   10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47
chain bonds :
3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21
21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46
46-47
exact/norm bonds :
1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27
27-28 28-29
29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
46-48

G1:[*1],[*2]

G2:[*3],[*4]

Connectivity :
1:3 X maximum RC ring/chain   2:3 X maximum RC ring/chain   3:3 X maximum RC

36

ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
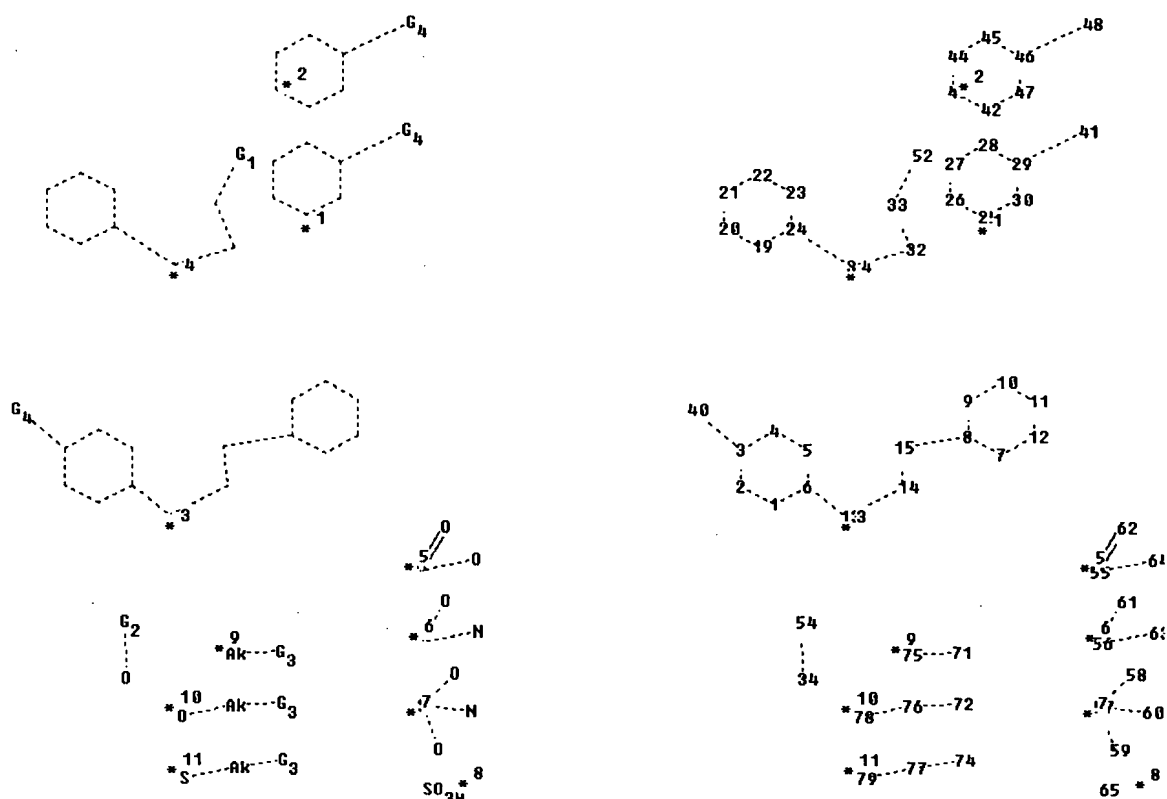54:CLASS

L6   STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation:
Uploading L6.str

chain nodes :
13　14　15　31　32　33　34　40　41　48　52　54　55　56　57　58　59　61　62　64　65
71　72　74　75　76　77　78　79
ring nodes :
1　2　3　4　5　6　7　8　9　10　11　12　19　20　21　22　23　24　25　26　27　28　29
30　42　43　44　45　46　47
ring/chain nodes :
60　63
chain bonds :
3-40　6-13　8-15　13-14　14-15　24-31　29-41　31-32　32-33　33-52　34-54　46-48
55-62　55-64　56-61　56-63　57-58　57-59　57-60　71-75　72-76　74-77　76-78　77-79
ring bonds :
1-2　1-6　2-3　3-4　4-5　5-6　7-8　7-12　8-9　9-10　10-11　11-12　19-20　19-24　20-
21
21-22　22-23　23-24　25-26　25-30　26-27　27-28　28-29　29-30　42-43　42-47　43-44
44-45　45-46
46-47
exact/norm bonds :
1-2　1-6　2-3　3-4　3-40　4-5　5-6　6-13　7-8　7-12　8-9　8-15　9-10　10-11　11-12
13-14　14-15　19-20　19-24　20-21　21-22　22-23　23-24　24-31　25-26　25-30　26-27
27-28　28-29
29-30　29-41　31-32　32-33　33-52　34-54　42-43　42-47　43-44　44-45　45-46　46-47
46-48　55-62
55-64　56-61　56-63　57-58　57-59　57-60　71-75　72-76　74-77　76-78　77-79

G1:[*1],[*2]

G2:[*3],[*4]

G3:[*5],[*6],[*7],[*8]

G4:[*9],[*10],[*11]

Connectivity :
1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS
55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS
63:CLASS 64:CLASS
65:CLASS 71:CLASS 72:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS
79:CLASS

L11   383 SEA FILE=BEILSTEIN SSS FUL L1 AND L3
L13   ·   5 SEA FILE=BEILSTEIN SUB=L11 SSS FUL L6

100.0% PROCESSED   383 ITERATIONS   5 ANSWERS
SEARCH TIME: 00.00.01

=> dup rem L26 L13
DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'ZCAPLUS' ENTERED AT 13:15:17 ON 01 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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